Registration

1. Express your interest by sending an e-mail message to sifisl@auth.gr

2. Pay the fee at the HSSTCM account at **PIRAEUS BANK (IBAN: GR74 XXXX XXXX XXXX XXXX XXXX 030).**
Do not forget to mention the participant's name and the word "workshop"

3. Send the bank transcription receipt as attachment to katsiki@auth.gr **Fees: 50 € (HSSTCM & FEMS members 30 €)**

Certificates of attendance: will be provided

Organizing Committee:

Assoc. Prof. Joseph Kioseoglou
Assoc. Prof. Maria Katsikini
School of Physics
Aristotle University of Thessaloniki

Prof. Elefterios Lidorikis
Assoc. Prof. Christina Lekka
Department of Materials Science and Engineering, University of Ioannina

Contact details:

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Faculty of Sciences
School of Physics

School of Physics
Faculty of Sciences
Aristotle University
of Thessaloniki

Hellenic Society for
the Science and
Technology of
Condensed Matter

Workshop

Computational Materials Science

Organized by the Hellenic Society for the Science and Technology of Condensed Matter under the auspices of the School of Physics

Saturday 14 & Sunday 15
December 2019
Thessaloniki, Greece

Program

A31 seminar room, 1st floor
Faculty of Sciences building
School of Physics

SPONSOR
Postgraduate Course Program
"Materials Physics and Technology"

Scope

The workshop on "Computational Materials Science" aims to provide an insight in selected fields in computational solid state physics, chemistry, materials science, surface science, catalysis, magnetism and nano-science. The term "Computational Materials Science" refers to a variety of theories, approaches and techniques of numerous implementations on:

- Bulk crystalline and amorphous materials
- Nanoscale 0D,1D, 2D structures
- Functional materials and Devices
- Extended defects, Surfaces and Interfaces
- Molecules, Macromolecules, Biomolecules

Saturday 14/12/2019

08:30 – 09:15 **Registration**

09:15 **Welcome and Introduction**

09:30 • **K. Kosmidis,** *Dr.,* Department of Physics, Aristotle Univ. of Thessaloniki, **Complex network approaches to bacterial gene regulation**

10:30 • **D.H. Tassis-C.A. Dimitriadis,** *Assoc. Prof.- Emer. Prof.,* School of Physics, Aristotle Univ. of Thessaloniki, **TCAD simulation and compact modelling of nano-scale transistors**

11:30 **Coffee break**

12:00 • **V.E. Raptis,** *Dr.,* Research Associate, Complex Systems Group Institute of Applied and Computational Mathematics Foundation for Research and Technology – Hellas, Heraklion, Crete, **Hierarchical approaches in molecular simulation of condensed matter and force-field development: from atomistic level to coarse graining.**

13:00 **Lunch break**

14:00 • **Ch. Lekka,** *Assoc. Prof., Department of Materials Science and Engineering, University of Ioannina* **On The Computational Design Of Ti- and Fe-Based Advanced Materials For Biomedical Applications**

15:00 • **E. Lidorikis**, *Prof.,* Department of Materials Science and Engineering, Univ. of Ioannina, **Multi-physics modeling and design of optoelectronic applications with graphene**

16:00 **Coffee break**

16:30 • **G.E. Froudakis,** *Prof.,* Department of Chemistry, University of Crete **Traditional theoretical methodologies vs novel machine learning techniques for addressing the gas storage problem**

17:30 • **E.C. Aifantis ,** *Emer. Prof.,* Laboratory of Mechanics and Materials School of Engineering, Aristotle Univ. of Thessaloniki, **Gradient Interatomic Potentials and Implications**

18:30 **End of the first day**

The lectures will include a short introduction with a review of fundamental principles and examples of recent work. Computational techniques that provide information and allow the study of materials from macro-to nano-scale, investigation of physical, chemical and biomedical properties, simulations of growth and synthesis methods and study of the properties of several types of bulk, functional and nanoscaled materials will be presented.

The workshop is aimed at M.Sc., Ph.D. Students, Post-Docs and researchers who wish to expand their knowledge in the field of "Computational Materials Science". Scientists, engineers and technicians working in research and education, who are interested in extending their knowledge in "Computational Materials Science", will also benefit.

All lecturers are experts in the field

Sunday 15/12/2019

09:30 • **K. Vyrsokinos,** *Assist. Prof.,* Department of Physics, Aristotle Univ. of Thessaloniki, **Photonics based High Performance Computing Systems**

10:30 • **H.M. Polatoglou**, *Prof.*, Department of Physics, Aristotle Univ. of Thessaloniki, **Introduction to Plasmonics and modeling with the Finite Element Method**

11:30 **Coffee break**

12:00 • **T.E. Karakasidis,** *Prof.,* Laboratory of Hydromechanics and Environmental Engineering, Department of Civil Engineering, University of Thessaly, **Size and surface effects in nano and mesoscale fluid flows investigated using particle methods**

13:00 **Lunch break**

14:00 • **D. Kechrakos**, *Assoc. Prof., Department of Education, School of Pedagogical and Technological Education (ASPETE), 14131 Athens, Greece*, **Modeling the Magnetic and Magnetotransport Properties of Nanostructured Materials**

15:00 **Coffee break**

15:30 • **P. Argyrakis,** *Emer. Prof.,* Department of Physics, Aristotle Univ. of Thessaloniki, **Smart algorithms for models of phase transitions in solids**

16:30 • **J. Kioseoglou,** *Assoc. Prof.,* Department of Physics, Aristotle Univ. of Thessaloniki, **Tailoring Properties of Nanoparticles through Atomic Scale Computational Design**

17:30 **End of workshop**

Workshops' language: *English*

The workshop will take place at the
School of Physics, Aristotle University of Thessaloniki Campus,
A31 Seminar room, 1st floor, Faculty of Sciences Building